



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 06:55 PM UTC

PDB ID : 9QBO / pdb_00009qbo
Title : Yeast 20S proteasome mutant: beta5_G128V (b5-propeptide in trans) in complex with MG132
Authors : Huber, E.M.; Heinemeyer, W.; Groll, M.
Deposited on : 2025-03-03
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

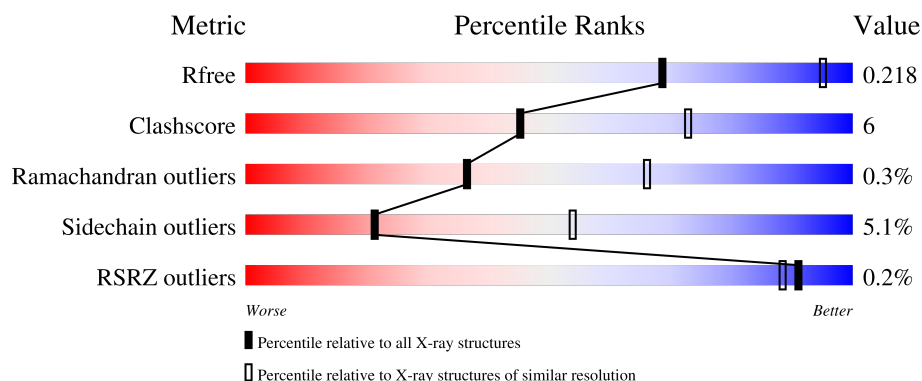
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div><div></div><div>95%</div><div>.</div></div>
1	O	250	<div><div></div><div>93%</div><div>6%</div></div>
2	B	258	<div><div></div><div>84%</div><div>10%</div><div>5%</div></div>
2	P	258	<div><div></div><div>%</div><div>84%</div><div>9%</div><div>5%</div></div>
3	C	254	<div><div></div><div>85%</div><div>7%</div><div>6%</div></div>





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Mol	Chain	Length	Quality of chain
3	Q	254	% 
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	231	
8	V	231	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	211	
11	Y	211	% 
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	195	
14	b	195	
15	f	4	
15	g	4	

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Mol	Chain	Length	Quality of chain
15	h	4	
15	i	4	
15	j	4	
15	k	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SO4	G	303	-	-	-	X
16	SO4	U	302	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 49864 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			
8	V	225	Total	C	N	O	S	0	0	0
			1712	1078	297	330	7			

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1640	1044	279	310	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	130	VAL	GLY	engineered mutation	UNP P30656
Y	130	VAL	GLY	engineered mutation	UNP P30656

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	1	0
			1832	1159	315	351	7			
13	a	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome subunit beta type-1.

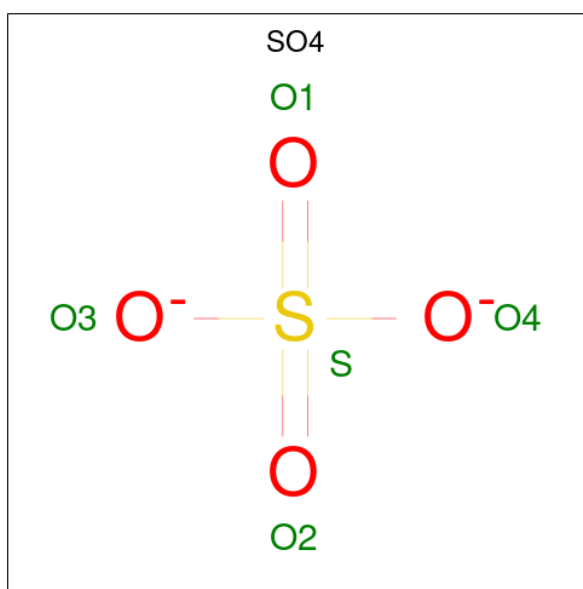
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			
14	b	195	Total	C	N	O	S	0	0	0
			1505	951	249	298	7			

- Molecule 15 is a protein called 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-C]PYRAZ

OLE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	f	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	g	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	h	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	i	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	j	4	Total	C	N	O	0	0	0
			41	30	4	7			
15	k	4	Total	C	N	O	0	0	0
			41	30	4	7			

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	O	S	0	0
			5	4	1		
16	G	1	Total	O	S	0	0
			5	4	1		
16	P	1	Total	O	S	0	0
			5	4	1		
16	U	1	Total	O	S	0	0
			5	4	1		

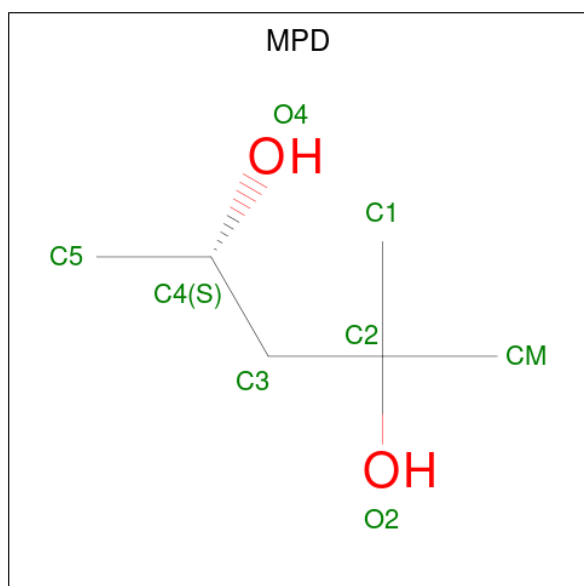
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total Mg 1 1	0	0
17	N	1	Total Mg 1 1	0	0

- Molecule 18 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

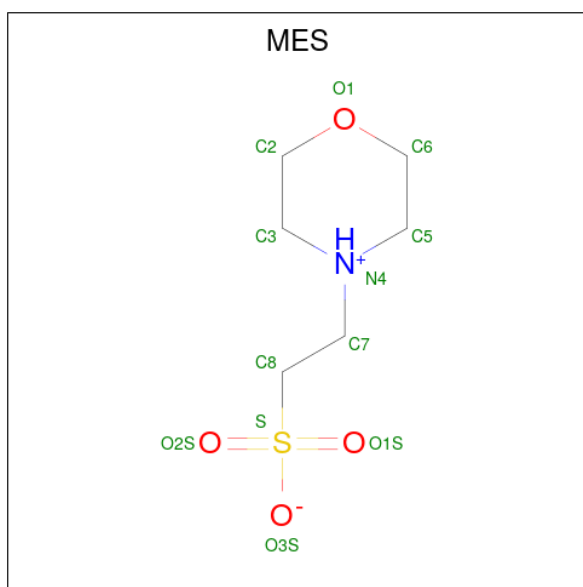
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	1	Total Cl 1 1	0	0
18	N	1	Total Cl 1 1	0	0
18	U	1	Total Cl 1 1	0	0
18	b	1	Total Cl 1 1	0	0

- Molecule 19 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	K	1	Total C O 8 6 2	0	0
19	a	1	Total C O 8 6 2	0	0

- Molecule 20 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	M	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
20	a	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

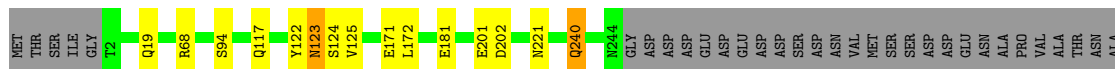
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	8	Total	O	0	0
			8	8		
21	B	10	Total	O	0	0
			10	10		
21	C	6	Total	O	0	0
			6	6		
21	D	4	Total	O	0	0
			4	4		
21	E	5	Total	O	0	0
			5	5		
21	F	10	Total	O	0	0
			10	10		
21	G	8	Total	O	0	0
			8	8		
21	H	8	Total	O	0	0
			8	8		
21	I	8	Total	O	0	0
			8	8		
21	J	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	K	3	Total O 3 3	0	0
21	L	11	Total O 11 11	0	0
21	M	15	Total O 15 15	0	0
21	N	9	Total O 9 9	0	0
21	O	2	Total O 2 2	0	0
21	P	6	Total O 6 6	0	0
21	Q	4	Total O 4 4	0	0
21	R	9	Total O 9 9	0	0
21	S	1	Total O 1 1	0	0
21	T	8	Total O 8 8	0	0
21	U	10	Total O 10 10	0	0
21	V	5	Total O 5 5	0	0
21	W	4	Total O 4 4	0	0
21	X	10	Total O 10 10	0	0
21	Y	7	Total O 7 7	0	0
21	Z	5	Total O 5 5	0	0
21	a	18	Total O 18 18	0	0
21	b	10	Total O 10 10	0	0
21	f	1	Total O 1 1	0	0
21	h	1	Total O 1 1	0	0
21	k	2	Total O 2 2	0	0



ASN
ALA
THR
THR
ASP
GLN
GLU
GLY
GLY
HIS
LEU
GLU

- Molecule 6: Probable proteasome subunit alpha type-7

Chain T:  79% 5% 16%

MET THR SER ILE ALA ASN GLY T2 Q19 R68 L77 R82 S94 Q117 Y122 N123 S124 G155 E171 L172 E181 E201 N221 Q240 Y244 GLY ASP ASP ASP GLU ASP ASP ASP ASP ASP ASP VAL MET SER SER ASP ASP GLU ASN ALA PRO VAL


ALA THR ASN GLY ALA ALA THR THR ASP GLN GLU ASP ILE HIS LEU GLU

- Molecule 7: Proteasome subunit alpha type-1

Chain G:  87% 8% . .

MET SER GLY ALA ALA ALA ALA SER ALA ALA G2 E13 F23 T26 L34 F64 R68 M72 V73 V74 P79 N83 N114 L115 R122 M125 K165 Q166 Q167 T171 L205 E208 R235 L236 Q242 ASP

- Molecule 7: Proteasome subunit alpha type-1

Chain U:  87% 8% . .


MET SER GLY ALA ALA ALA ALA SER ALA ALA G2 P12 E13 F23 T26 L34 T59 R63 I78 P79 N83 N114 L115 R122 M125 A159 K165 Q166 Q167 T171 L205 E208 K223 R235 L236 Q242 ASP

- Molecule 8: Proteasome subunit beta type-2

Chain H:  86% 10% . .

T2 R19 K33 L34 S38 A50 V55 L68 L80 Y97 L98 D104 P105 L110 F111 S112 I113 H114 T119 L125 S126 L127 I163 V164 N165 D166 G170 N194 V195 R196 L213 K214 E215 I223 E226 GLN VAL ASP ILE ALA


- Molecule 8: Proteasome subunit beta type-2

Chain V:  84% 11% . .

T2 R19 K33 L34 S38 A50 V55 L68 L80 L83 Y97 L98 D104 P105 I113 H114 T119 L125 S126 L127 S131 L132 I163 V164 N165 D166 L167 G170 N194 V195 R196 V212 L213 K214 E215 I223 E226 GLN VAL

ASP
ILE
THR
ALA

- Molecule 9: Proteasome subunit beta type-3

Chain I:  86% 12% .

MET S1 N7 G8 G9 I10 V20 G29 G34 N37 K41 A56 T57 D59 N71 E77 P101 P118 F123 I126 G127 C128 A141 E150 L171 R176 W182 G183 R197 K200 M201 R202 Q203 D204

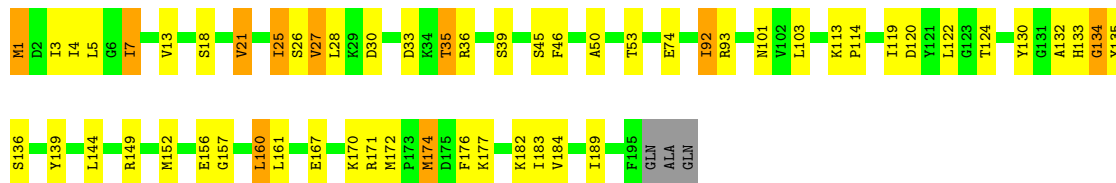
- Molecule 9: Proteasome subunit beta type-3

Chain W:  87% 11% .



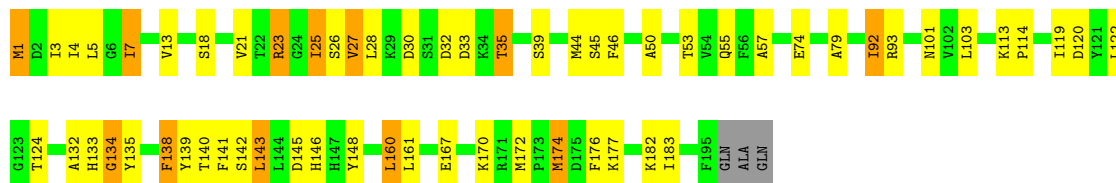
- Molecule 10: Proteasome subunit beta type-4

Chain J:  70% 24% 5% .



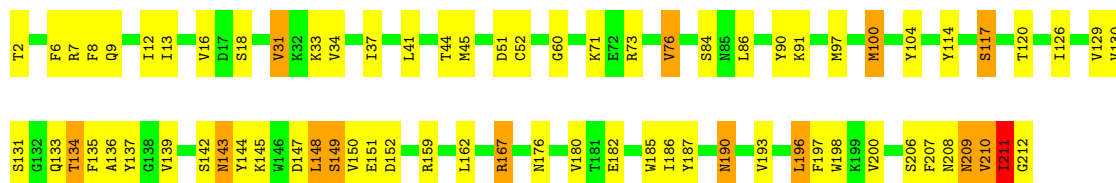
- Molecule 10: Proteasome subunit beta type-4

Chain X:  68% 24% 6% .



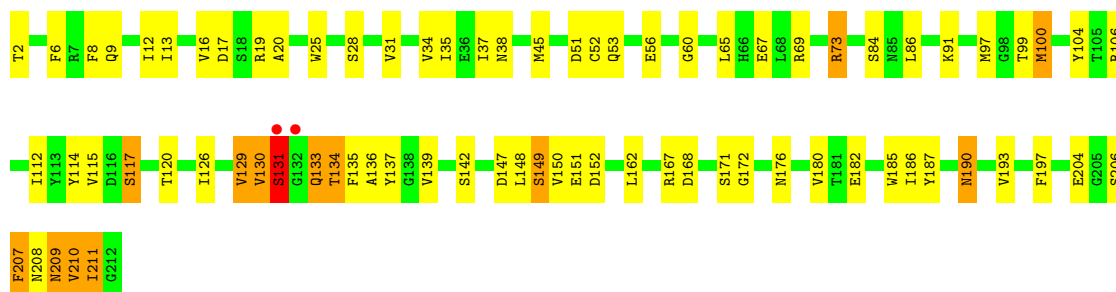
- Molecule 11: Proteasome subunit beta type-5

Chain K:  65% 28% 6% .

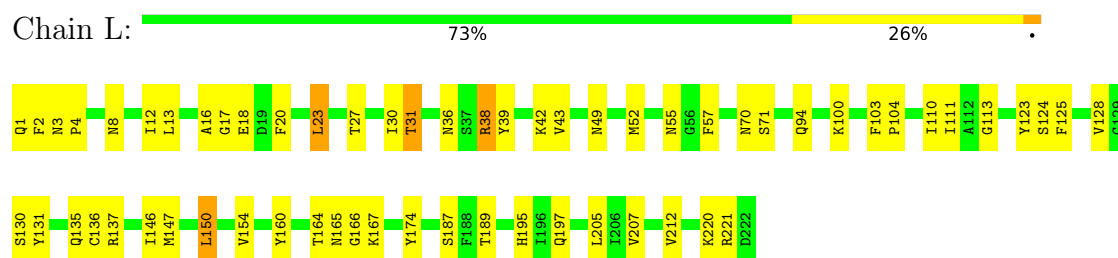


- Molecule 11: Proteasome subunit beta type-5

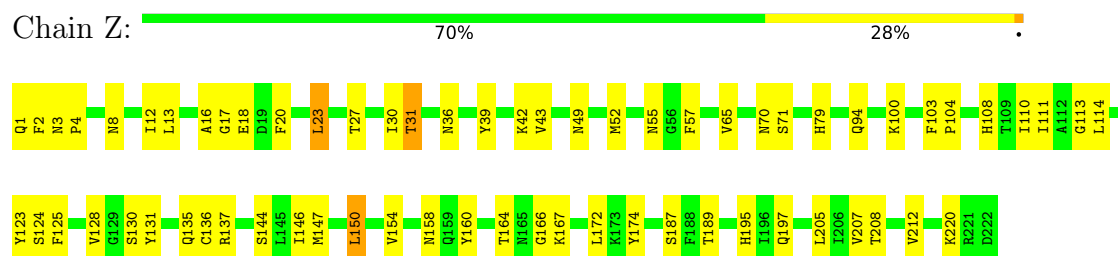
Chain Y:  63% 30% 6% .



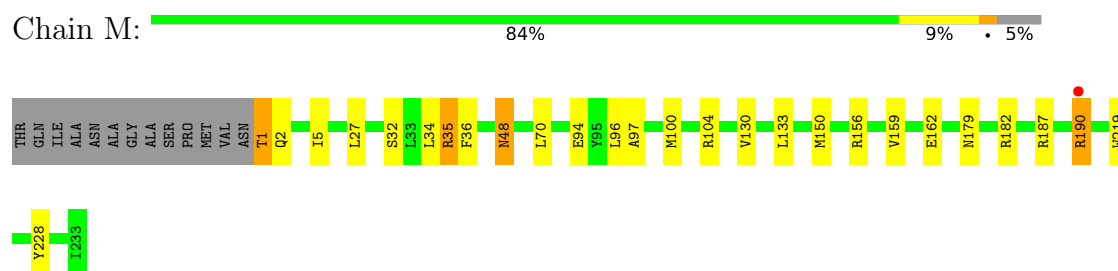
- Molecule 12: Proteasome subunit beta type-6



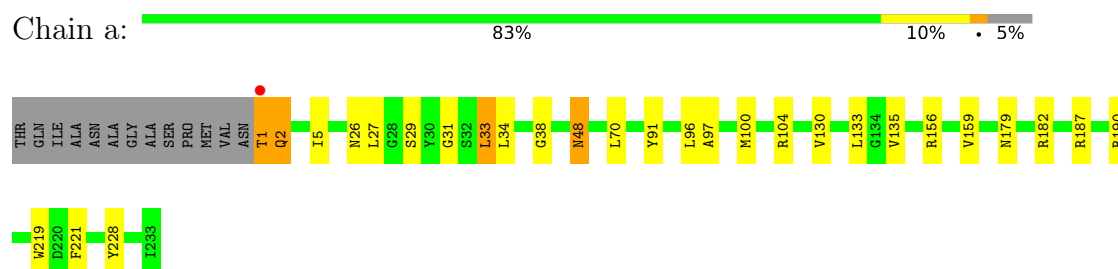
- Molecule 12: Proteasome subunit beta type-6



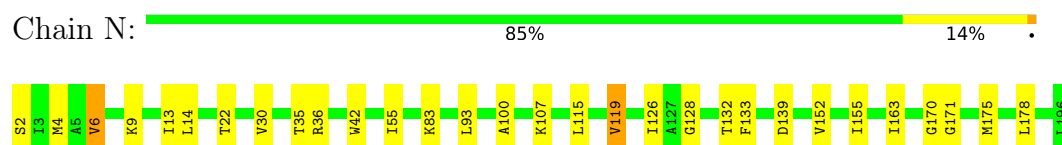
- Molecule 13: Proteasome subunit beta type-7




- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1

Chain b:  84% 15% .



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain f:  25% 25% 50%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain g:  50% 25% 25%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain h:  50% 25% 25%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain i:  25% 25% 50%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain j:  50% 25% 25%



• Molecule 15: 3-PYRIDIN-4-YL-2,4-DIHYDRO-INDENO[1,2-.C.]PYRAZOLE

Chain k:  50% 25% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.19Å 298.96Å 146.78Å 90.00° 112.98° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.80) 97.8 (15.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.174 , 0.212 0.170 , 0.218	Depositor DCC
R_{free} test set	13019 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	1.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	49864	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A1I48, SO4, MPD, MES, P6S, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.03	0/1952	1.42	0/2642
1	O	1.03	0/1952	1.43	0/2642
2	B	1.04	0/1934	1.44	0/2618
2	P	1.04	0/1934	1.44	0/2618
3	C	1.04	0/1910	1.47	0/2586
3	Q	1.05	0/1910	1.47	0/2586
4	D	1.04	0/1837	1.48	0/2475
4	R	1.04	0/1837	1.48	0/2475
5	E	1.04	0/1800	1.44	2/2433 (0.1%)
5	S	1.04	0/1800	1.45	2/2433 (0.1%)
6	F	1.03	0/1932	1.45	0/2609
6	T	1.04	0/1932	1.46	2/2609 (0.1%)
7	G	1.02	0/1945	1.42	0/2634
7	U	1.03	0/1945	1.42	0/2634
8	H	1.01	0/1743	1.40	0/2363
8	V	1.02	0/1743	1.40	0/2363
9	I	1.03	0/1611	1.41	2/2174 (0.1%)
9	W	1.04	0/1611	1.42	2/2174 (0.1%)
10	J	0.96	0/1589	1.36	2/2142 (0.1%)
10	X	0.94	0/1589	1.33	2/2142 (0.1%)
11	K	0.96	0/1677	1.37	0/2269
11	Y	0.95	0/1677	1.39	0/2269
12	L	0.95	0/1795	1.35	0/2420
12	Z	0.95	0/1795	1.35	0/2420
13	M	1.05	0/1866	1.42	2/2528 (0.1%)
13	a	1.03	0/1855	1.40	0/2514
14	N	1.01	0/1534	1.40	1/2077 (0.0%)
14	b	1.01	0/1534	1.40	1/2077 (0.0%)
15	f	0.74	0/15	0.82	0/19
15	g	1.79	0/15	1.34	0/19
15	h	0.79	0/15	0.86	0/19
15	i	0.75	0/15	0.70	0/19

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	j	0.85	0/15	0.81	0/19
15	k	0.86	0/15	0.96	0/19
All	All	1.02	0/50329	1.42	18/68040 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	f	0	1
15	g	0	1
15	h	0	1
15	i	0	1
15	j	0	1
15	k	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	190[A]	ARG	CA-C-O	8.32	130.02	119.95
13	M	190[B]	ARG	CA-C-O	8.32	130.02	119.95
9	I	183	GLY	CA-C-O	-5.76	118.47	122.22
9	W	183	GLY	CA-C-O	-5.70	118.34	122.45
10	X	134	GLY	CA-C-N	5.35	127.45	120.28

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	f	3	LEU	Peptide
15	g	3	LEU	Peptide
15	h	3	LEU	Peptide
15	i	3	LEU	Peptide
15	j	3	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	7	0
1	O	1915	0	1929	15	0
2	B	1904	0	1904	26	0
2	P	1904	0	1904	20	0
3	C	1881	0	1895	15	0
3	Q	1881	0	1895	15	0
4	D	1813	0	1797	11	0
4	R	1813	0	1797	12	0
5	E	1773	0	1775	20	0
5	S	1773	0	1775	20	0
6	F	1892	0	1883	13	0
6	T	1892	0	1883	6	0
7	G	1907	0	1901	13	0
7	U	1907	0	1901	14	0
8	H	1712	0	1709	26	0
8	V	1712	0	1709	27	0
9	I	1581	0	1574	27	0
9	W	1581	0	1574	24	0
10	J	1561	0	1569	61	0
10	X	1561	0	1569	67	0
11	K	1640	0	1591	69	0
11	Y	1640	0	1591	70	0
12	L	1757	0	1711	45	0
12	Z	1757	0	1711	47	0
13	M	1832	0	1845	21	0
13	a	1824	0	1832	22	0
14	N	1505	0	1471	19	0
14	b	1505	0	1471	18	0
15	f	41	0	21	1	0
15	g	41	0	21	1	0
15	h	41	0	21	0	0
15	i	41	0	21	1	0
15	j	41	0	21	0	0
15	k	41	0	21	0	0
16	B	5	0	0	0	0
16	G	5	0	0	1	0
16	P	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	U	5	0	0	0	0
17	G	1	0	0	0	0
17	N	1	0	0	0	0
18	G	1	0	0	0	0
18	N	1	0	0	0	0
18	U	1	0	0	0	0
18	b	1	0	0	0	0
19	K	8	0	14	3	0
19	a	8	0	14	0	0
20	M	12	0	13	1	0
20	a	12	0	13	0	0
21	A	8	0	0	0	0
21	B	10	0	0	0	0
21	C	6	0	0	0	0
21	D	4	0	0	0	0
21	E	5	0	0	0	0
21	F	10	0	0	0	0
21	G	8	0	0	0	0
21	H	8	0	0	0	0
21	I	8	0	0	0	0
21	J	6	0	0	0	0
21	K	3	0	0	0	0
21	L	11	0	0	0	0
21	M	15	0	0	0	0
21	N	9	0	0	0	0
21	O	2	0	0	0	0
21	P	6	0	0	0	0
21	Q	4	0	0	0	0
21	R	9	0	0	0	0
21	S	1	0	0	0	0
21	T	8	0	0	0	0
21	U	10	0	0	0	0
21	V	5	0	0	0	0
21	W	4	0	0	0	0
21	X	10	0	0	1	0
21	Y	7	0	0	0	0
21	Z	5	0	0	0	0
21	a	18	0	0	1	0
21	b	10	0	0	0	0
21	f	1	0	0	0	0
21	h	1	0	0	0	0
21	k	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	49864	0	49275	584	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 584 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:31:THR:HG22	12:L:36:ASN:HD21	1.11	1.13
12:Z:31:THR:HG22	12:Z:36:ASN:HD21	0.93	1.05
11:Y:129:VAL:HG22	11:Y:134:THR:HG23	1.39	1.02
11:K:167:ARG:NH2	9:W:182:TRP:HH2	1.57	1.01
12:Z:31:THR:HG22	12:Z:36:ASN:ND2	1.75	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	60
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	60
2	B	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	25
2	P	242/258 (94%)	234 (97%)	4 (2%)	4 (2%)	7	25
3	C	238/254 (94%)	232 (98%)	4 (2%)	2 (1%)	16	44
3	Q	238/254 (94%)	232 (98%)	4 (2%)	2 (1%)	16	44
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
5	E	229/234 (98%)	223 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	S	229/234 (98%)	223 (97%)	6 (3%)	0	100	100
6	F	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
6	T	241/288 (84%)	236 (98%)	5 (2%)	0	100	100
7	G	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
7	U	239/252 (95%)	236 (99%)	3 (1%)	0	100	100
8	H	223/231 (96%)	218 (98%)	5 (2%)	0	100	100
8	V	223/231 (96%)	218 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	209/211 (99%)	200 (96%)	6 (3%)	3 (1%)	9	30
11	Y	209/211 (99%)	200 (96%)	5 (2%)	4 (2%)	6	22
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
13	a	231/246 (94%)	225 (97%)	6 (3%)	0	100	100
14	N	193/195 (99%)	190 (98%)	3 (2%)	0	100	100
14	b	193/195 (99%)	189 (98%)	4 (2%)	0	100	100
15	f	1/4 (25%)	1 (100%)	0	0	100	100
15	g	1/4 (25%)	1 (100%)	0	0	100	100
15	h	1/4 (25%)	1 (100%)	0	0	100	100
15	i	1/4 (25%)	1 (100%)	0	0	100	100
15	j	1/4 (25%)	1 (100%)	0	0	100	100
15	k	1/4 (25%)	1 (100%)	0	0	100	100
All	All	6285/6632 (95%)	6127 (98%)	137 (2%)	21 (0%)	36	66

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN

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Mol	Chain	Res	Type
11	K	207	PHE
11	K	210	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	50	81
1	O	209/209 (100%)	205 (98%)	4 (2%)	50	81
2	B	203/216 (94%)	197 (97%)	6 (3%)	36	72
2	P	203/216 (94%)	197 (97%)	6 (3%)	36	72
3	C	212/226 (94%)	202 (95%)	10 (5%)	23	57
3	Q	212/226 (94%)	202 (95%)	10 (5%)	23	57
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	53
4	R	194/215 (90%)	185 (95%)	9 (5%)	24	58
5	E	190/193 (98%)	183 (96%)	7 (4%)	30	65
5	S	190/193 (98%)	183 (96%)	7 (4%)	30	65
6	F	201/239 (84%)	189 (94%)	12 (6%)	17	47
6	T	201/239 (84%)	191 (95%)	10 (5%)	22	54
7	G	206/210 (98%)	197 (96%)	9 (4%)	25	59
7	U	206/210 (98%)	197 (96%)	9 (4%)	25	59
8	H	184/189 (97%)	176 (96%)	8 (4%)	26	60
8	V	184/189 (97%)	173 (94%)	11 (6%)	17	47
9	I	172/173 (99%)	169 (98%)	3 (2%)	53	83
9	W	172/173 (99%)	169 (98%)	3 (2%)	53	83
10	J	173/175 (99%)	160 (92%)	13 (8%)	12	37
10	X	173/175 (99%)	159 (92%)	14 (8%)	11	33
11	K	169/169 (100%)	145 (86%)	24 (14%)	3	12
11	Y	169/169 (100%)	147 (87%)	22 (13%)	4	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	185/185 (100%)	174 (94%)	11 (6%)	18	48
12	Z	185/185 (100%)	172 (93%)	13 (7%)	14	40
13	M	200/208 (96%)	193 (96%)	7 (4%)	32	67
13	a	199/208 (96%)	191 (96%)	8 (4%)	28	63
14	N	161/161 (100%)	154 (96%)	7 (4%)	26	60
14	b	161/161 (100%)	154 (96%)	7 (4%)	26	60
15	f	2/2 (100%)	0	2 (100%)	0	0
15	g	2/2 (100%)	2 (100%)	0	100	100
15	h	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	i	2/2 (100%)	0	2 (100%)	0	0
15	j	2/2 (100%)	1 (50%)	1 (50%)	0	0
15	k	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	5329/5548 (96%)	5058 (95%)	271 (5%)	21	54

5 of 271 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Y	151	GLU
12	Z	31	THR
14	b	22	THR
11	K	149	SER
11	K	142	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

Mol	Chain	Res	Type
5	S	99	ASN
9	W	44	HIS
5	S	151	ASN
7	U	83	ASN
10	X	78	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	A1I48	k	4	15,14	12,14,15	1.50	1 (8%)	10,18,20	1.34	1 (10%)
15	A1I48	f	4	15,8	12,14,15	1.48	1 (8%)	10,18,20	1.41	2 (20%)
15	A1I48	h	4	15,14	12,14,15	1.52	1 (8%)	10,18,20	1.36	1 (10%)
15	A1I48	g	4	15,11	12,14,15	0.75	0	10,18,20	1.49	2 (20%)
15	A1I48	j	4	15,11	12,14,15	1.42	1 (8%)	10,18,20	1.47	2 (20%)
15	A1I48	i	4	15,8	12,14,15	1.47	1 (8%)	10,18,20	1.44	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	A1I48	k	4	15,14	-	4/15/18/20	-
15	A1I48	f	4	15,8	-	4/15/18/20	-
15	A1I48	h	4	15,14	-	4/15/18/20	-
15	A1I48	g	4	15,11	-	4/15/18/20	-
15	A1I48	j	4	15,11	-	5/15/18/20	-
15	A1I48	i	4	15,8	-	4/15/18/20	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	h	4	A1I48	CA-N2	-4.75	1.33	1.47
15	k	4	A1I48	CA-N2	-4.70	1.34	1.47
15	f	4	A1I48	CA-N2	-4.60	1.34	1.47
15	i	4	A1I48	CA-N2	-4.54	1.34	1.47
15	j	4	A1I48	CA-N2	-4.31	1.35	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	4	A1I48	C22-OG1-CB	-3.05	111.00	115.27
15	h	4	A1I48	CB-CA-N2	-2.92	95.08	114.17
15	i	4	A1I48	CB-CA-N2	-2.81	95.78	114.17
15	f	4	A1I48	CB-CA-N2	-2.77	96.06	114.17
15	k	4	A1I48	CB-CA-N2	-2.73	96.32	114.17

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	f	4	A1I48	O23-C22-OG1-CB
15	f	4	A1I48	O-C-CA-CB
15	g	4	A1I48	O23-C22-OG1-CB
15	g	4	A1I48	C-CA-CB-CG2
15	g	4	A1I48	C-CA-CB-OG1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	f	4	A1I48	1	0
15	g	4	A1I48	1	0
15	i	4	A1I48	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	MPD	a	302	-	7,7,7	0.14	0	9,10,10	0.36	0
20	MES	a	301	-	12,12,12	0.65	0	15,16,16	0.39	0
16	SO4	U	302	-	4,4,4	0.55	0	6,6,6	0.15	0
16	SO4	G	303	-	4,4,4	0.60	0	6,6,6	0.22	0
16	SO4	P	301	-	4,4,4	0.34	0	6,6,6	0.08	0
19	MPD	K	301	-	7,7,7	0.17	0	9,10,10	0.46	0
16	SO4	B	301	-	4,4,4	0.34	0	6,6,6	0.08	0
20	MES	M	301	-	12,12,12	0.66	0	15,16,16	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	MPD	K	301	-	-	2/5/5/5	-
19	MPD	a	302	-	-	0/5/5/5	-
20	MES	M	301	-	-	4/6/14/14	0/1/1/1
20	MES	a	301	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	K	301	MPD	C2-C3-C4-O4
19	K	301	MPD	C2-C3-C4-C5
20	M	301	MES	C7-C8-S-O3S
20	M	301	MES	N4-C7-C8-S
20	M	301	MES	C7-C8-S-O1S

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	303	SO4	1	0
19	K	301	MPD	3	0
20	M	301	MES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.62	0 100 100	56, 72, 105, 140	0
1	O	250/250 (100%)	-0.64	1 (0%) 88 84	59, 79, 120, 156	0
2	B	244/258 (94%)	-0.44	1 (0%) 88 84	54, 76, 128, 181	0
2	P	244/258 (94%)	-0.55	2 (0%) 82 75	60, 79, 123, 164	0
3	C	240/254 (94%)	-0.59	0 100 100	58, 81, 141, 156	0
3	Q	240/254 (94%)	-0.48	2 (0%) 82 75	60, 91, 159, 182	0
4	D	235/260 (90%)	-0.62	0 100 100	60, 82, 116, 132	0
4	R	235/260 (90%)	-0.59	0 100 100	61, 85, 120, 139	0
5	E	231/234 (98%)	-0.55	0 100 100	62, 85, 122, 158	0
5	S	231/234 (98%)	-0.51	0 100 100	63, 93, 135, 149	0
6	F	243/288 (84%)	-0.67	0 100 100	55, 77, 119, 144	0
6	T	243/288 (84%)	-0.59	0 100 100	55, 84, 129, 141	0
7	G	241/252 (95%)	-0.69	0 100 100	53, 71, 106, 154	0
7	U	241/252 (95%)	-0.68	0 100 100	58, 75, 110, 144	0
8	H	225/231 (97%)	-0.67	1 (0%) 88 84	51, 67, 102, 156	0
8	V	225/231 (97%)	-0.65	1 (0%) 88 84	53, 70, 104, 171	0
9	I	204/205 (99%)	-0.77	0 100 100	51, 68, 93, 119	0
9	W	204/205 (99%)	-0.83	0 100 100	52, 70, 98, 124	0
10	J	195/198 (98%)	-0.71	0 100 100	51, 75, 106, 132	0
10	X	195/198 (98%)	-0.76	0 100 100	55, 76, 107, 135	0
11	K	211/211 (100%)	-0.61	0 100 100	55, 75, 116, 139	0
11	Y	211/211 (100%)	-0.62	2 (0%) 81 74	60, 75, 119, 134	0
12	L	222/222 (100%)	-0.76	0 100 100	54, 72, 110, 122	0
12	Z	222/222 (100%)	-0.78	0 100 100	55, 72, 110, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.68	1 (0%) 88 84	52, 68, 93, 109	1 (0%)
13	a	233/246 (94%)	-0.77	1 (0%) 88 84	50, 67, 91, 104	0
14	N	195/195 (100%)	-0.81	0 100 100	48, 62, 92, 115	0
14	b	195/195 (100%)	-0.77	0 100 100	51, 64, 94, 119	0
15	f	2/4 (50%)	0.08	0 100 100	84, 84, 84, 84	0
15	g	2/4 (50%)	-0.50	0 100 100	76, 76, 76, 78	0
15	h	2/4 (50%)	-0.59	0 100 100	70, 70, 70, 73	0
15	i	2/4 (50%)	0.44	0 100 100	90, 90, 90, 91	0
15	j	2/4 (50%)	-0.58	0 100 100	82, 82, 82, 83	0
15	k	2/4 (50%)	-0.75	0 100 100	66, 66, 66, 70	0
All	All	6350/6632 (95%)	-0.65	12 (0%) 91 88	48, 75, 120, 182	1 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	218	GLY	3.7
3	Q	50	LEU	3.4
13	a	1	THR	3.1
13	M	190[A]	ARG	3.1
8	H	223	ILE	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	A1I48	j	4	15/16	0.96	0.08	68,79,83,83	0
15	A1I48	k	4	15/16	0.96	0.08	64,68,75,75	0
15	A1I48	h	4	15/16	0.97	0.08	58,66,77,83	0
15	A1I48	i	4	15/16	0.97	0.08	65,73,79,85	0
15	A1I48	f	4	15/16	0.97	0.09	65,76,84,86	0
15	A1I48	g	4	15/16	0.97	0.07	70,75,77,80	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	SO4	U	302	5/5	0.75	0.46	20,20,20,20	0
20	MES	M	301	12/12	0.75	0.17	135,172,177,179	0
16	SO4	G	303	5/5	0.79	0.44	20,20,20,20	0
18	CL	N	202	1/1	0.80	0.35	30,30,30,30	0
18	CL	b	201	1/1	0.82	0.40	30,30,30,30	0
20	MES	a	301	12/12	0.85	0.13	141,166,174,180	0
19	MPD	a	302	8/8	0.87	0.16	109,120,134,137	0
19	MPD	K	301	8/8	0.92	0.14	90,99,105,105	0
18	CL	U	301	1/1	0.95	0.06	101,101,101,101	0
18	CL	G	302	1/1	0.95	0.08	93,93,93,93	0
16	SO4	P	301	5/5	0.96	0.12	127,131,143,145	0
16	SO4	B	301	5/5	0.96	0.16	123,128,147,161	0
17	MG	G	301	1/1	0.97	0.06	94,94,94,94	0
17	MG	N	201	1/1	0.97	0.11	125,125,125,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.